Theoretical formalism to understand the role of strain in the tailoring of hole masses in p-type $In_xGa_{1-x}As$ (on GaAs substrates) and $In_{0.53+x}Ga_{0.47-x}As$ (on InP substrates) modulation-doped field-effect transistors

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Recently, experimental studies have suggested that strained p-channel modulation-doped field-effect transistors (MODFET's) display enhanced characteristics due to a decrease in hole masses. In this letter, we examine the potential of using biaxial compressive strain to lower the effective mass of the hole gas. The Kohn–Luttinger Hamiltonian is used to describe the hole states in a strained channel. Using this, the Schrödinger equation is solved self-consistently with the Poisson equation. The coupling between light- and heavy-hole states is found to be critical to get accurate properties of the hole gas. A decrease in the effective hole mass of more than three times is found at low temperatures in the presence of the biaxial strain. The theoretical technique described here is not variational in nature and can be applied to an arbitrarily shaped confining potential profile with different material parameters across interfaces. This technique should be quite useful in designing and understanding strained p-MODFET devices.

Epitaxial crystal growth techniques such as molecular beam epitaxy (MBE) have made possible the fabrication of high-quality heterostructure-based devices such as modulation-doped field-effect transistors (MODFET's). n-type MODFET's have shown exceptional performance. The ease in material control in MBE growth has also allowed the fabrication of strained n-MODFET's which have shown even better performance.[1] p-MODFET's have not been pursued as actively primarily because of the high hole masses and low hole mobilities. However, the availability of high-quality p-MODFET's is clearly of value for complementary logic. p-MODFET studies have been carried out by Tiwari and Wang[2] who considered the lattice-matched AlGaAs/GaAs system, by Drummond *et al.*[3] who examined the strained GaAs/InGaAs system, and Lee *et al.*,[4] who showed remarkable performance in the AlGaAs/InGaAs system. However, a model which can accurately describe the properties in a strained p-type MODFET has not been presented. In order to model a strained p-type MODFET, one must solve the Poisson equation self-consistently with the Schrödinger equation. A Hamiltonian must be chosen which is capable of accurately representing the full heavy- and light-hole system in the presence of biaxial strain.

In this letter, we use the Kohn–Luttinger Hamiltonian to describe the valence-band states with and without the presence of strain. We show that while it is difficult to avoid the heavy-hole mass of the two-dimensional hole gas in lattice-matched p-MODFET's, one can obtain lighter hole masses in strained channels. We examine this possibility in p-MODFET's lattice matched to GaAs and InP substrates. Biaxial compressive strain is produced in the channel by increasing the In composition, x($x = 0$ is the lattice-matched system on a GaAs substrate and $x = 0.53$ is the lattice matched system on an InP substrate). As will be shown, biaxial compressive strain, which is present in the cases which we model in this letter, reduces the effective hole mass while for small strains, biaxial tensile strain increases the effective hole mass.

In the case of the n-MODFET, the effect of adding excess In in the channel of the device decreases the electron mass, but the net change is only around 10% for 10% excess In concentration.[5] The solution for the n-MODFET is relatively simple since one only has to solve the single-band Schrödinger equation in one dimension self-consistently with the Poisson equation. For hole states, however, it is well known that there are four states which describe the top of the valence band, and that the coupling between these states is quite critical. These four states and the coupling between them are adequately described by the Kohn–Luttinger Hamiltonian.[6] We solve the Schrödinger equation as a numerical finite difference eigenvalue problem, not variationally as other workers have done in the past. Because of this, we are free to include a spatial variation of the Luttinger parameters in order to model the bands as they pass into different material layers. We included three sets of parameters, one set for the barrier material (AlGaAs or AlInAs), one set for the strained well, and a third set for the buffer material below the well. For our simulations, we used the Luttinger parameters given by Lawaetz,[7] taking an average of parameters in the case of alloys. A small uncertainty in the calculations may be introduced here because these parameters are not very well known, and the differences in parameters from one material to another may not be completely consistent.

Solution of the Schrödinger equation yields the dispersion relation in the k_x-k_y plane for the heavy- and light-hole bands. Integrating the two-dimensional dispersion relation yields the density of states in each band. Integration of the

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density of states times the Fermi distribution function will give the total occupation in each subband.

The potential profile in the growth direction of the device is determined from the self-consistent solution of the Schrödinger equation and the Poisson equation. The charge profile in the Poisson equation is taken to be

$$\rho(z) = N_d(z) - N_a(z) - n_{\text{free}}(z) + p_{\text{free}}(z) - \sum_i p_i \phi_i^*(z)\phi_i(z). \quad (1)$$

Here, N_a and N_d represent the doping levels, n_{free} and p_{free} are the free electron and hole concentrations which are calculated using Fermi–Dirac statistics, and the sum is over i two dimensionally confined bands in which the hole concentrations are p_i. Implicit in Eq. (1) is the idea that each band can be characterized by a wave function $\phi_i(z)$ whose spatial variation does not strongly depend upon k, i.e.,

$$\phi_i(z,\mathbf{k}=0) \approx \phi_i(z,\mathbf{k}). \quad (2)$$

Our calculations show that while this assumption is not always valid, especially at positions where two bands either cross or come close to one another, it does yield good results for the net quantum-confined charge distribution through real space.

The effect of the biaxial strain is to cause a splitting in the heavy- and light-hole band gaps and is given by Ref. 8.

$$\text{heavy hole: } E_{\text{HH}} = E_0 + \tfrac{1}{2}\delta_{\text{sh}} - \delta_{\text{hy}}, \quad (3)$$

$$\text{light hole: } E_{\text{LH}} = E_0 - \tfrac{1}{2}\delta_{\text{sh}} - \delta_{\text{hy}}, \quad (4)$$

where δ_{sh} and δ_{hy} are the shear and hydrostatic portions of the change in the band energies from the unstrained band energy position E_0, and are given by

$$\delta_{\text{sh}} = -2b[(c_{11} + 2c_{12})/c_{11}]\epsilon, \quad (5)$$

$$\delta_{\text{hy}} = -2a[(c_{11} - c_{12})/c_{11}]\epsilon. \quad (6)$$

Here c_{11} and c_{12} are the elastic parameters of the channel material, ϵ is the strain in the parallel direction, and a and b are the material deformation potentials. Evaluation of these equations for $In_xGa_{1-x}As$ yields shifts of -5.96ϵ for the heavy-hole band and -12.4ϵ for the light-hole band.[8] The splitting between the heavy- and light-hole states is included in the diagonal terms of the Kohn–Luttinger Hamiltonian. The splitting between the HH and LH states will alter the band to band coupling and, consequently, will change the parallel effective mass. Our results show that this effect can be rather significant. By taking advantage of this effect, one can obtain much lighter effective masses in the upper hole bands.

Two important observations about our technique lead us to expect certain trends in the results. The first is that due to the off-diagonal matrix elements in the Kohn–Luttinger Hamiltonian, the heavy- and the light-hole states will interact strongly. Thus, the heavy- and the light-hole masses in the direction parallel to the interface depend upon $V(z)$, the potential profile perpendicular to the interface. This does not happen in n-MODFET's, and is solely a consequence of heavy hole-light hole coupling. The second observation is that because we are strongly breaking inversion symmetry, both because of an asymmetric potential profile and because of the fact that we are using different Luttinger parameters above and below the two-dimensional hole gas, we will expect a large lifting of the degeneracy between the spin up and spin down states, Kramer's degeneracy.

In Fig. 1 we show some typical results for the hole dispersion relations in the strained channel for (a) $x = 0$ (no strain) and (b) $x = 0.12$ (0.84% strain) for $V_g = 0.0$ V at room temperature. Note that each pair (spin up and spin down) of heavy- and light-hole states is no longer degenerate except at $\mathbf{k} = 0$. Also shown are the corresponding valence-band profiles and the subband levels in the channel. Due to strain-induced splitting of the valence band, the heavy- and the light-hole states will see a different effective potential profile. These potentials are represented by dotted lines in the figure. Note that since the strain increases the depth of the well in which the holes reside, there will be stronger confinement. Examination of the dispersion relations in Fig. 2 clearly shows that in the presence of strain, the hole states are much better behaved and much lighter.

In Table I we show some of the quantitative information which we calculated for the GaAs-based p-MODFET's. We get essentially similar results for the InP-based systems. Shown are the energies of the various subbands, the occupation of each subband, the density of states effective mass of each subband, the total two-dimensionally confined charge, and the average effective mass. Important points noted are: (i) Large reduction of heavy-hole mass (by a factor of 3.7 at liquid nitrogen temperatures and a factor of 1.7 at room temperature), and (ii) much stronger charge confinement in a strained channel.

As the temperature is decreased, the shapes of the bands do not change very much, but the density of states effective masses may. This is because the holes become more crowded

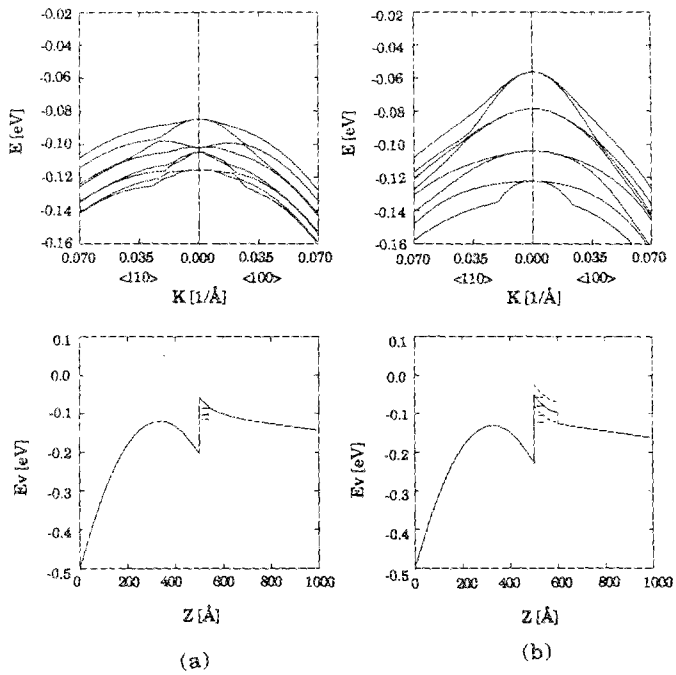

FIG 1. Hole dispersion relations and potential profiles resulting from the solution of the charge control model at 300 K with $V_g = 0$. Case (a) lattice-matched system, case (b) 12% excess indium in the channel. In both cases, the Fermi energy is at 0.0 eV.

TABLE I. Simulation results showing the occupation density, effective mass, energy, and state type of the top eight subbands in a lattice-matched and a strained p-type MODFET at 300 K and 77 K.

		GaAs channel				$In_{0.12}Ga_{0.88}As$ channel			
Temp. (K)	subband No.	n_s 10^{11}	m^*_{dos}	$E_n - E_F$ (meV)	state	n_s 10^{11}	m^*_{dos}	$E_n - E_F$ (meV)	state
300	0	1.19	0.601	− 84.8	HH0	1.49	0.257	− 56.4	HH0
	1	0.95	0.481	− 84.8	HH0	1.15	0.199	− 56.4	HH0
	2	0.70	0.686	− 102.0	LH0	0.86	0.342	− 78.6	HH1
	3	0.64	0.624	− 102.0	LH0	0.79	0.313	− 78.6	HH1
	4	0.45	0.485	− 105.0	HH1	0.53	0.561	− 104.0	HH2
	5	0.43	0.463	− 105.0	HH1	0.39	0.406	− 104.0	HH2
	6	0.35	0.566	− 116.0	HH2	0.27	0.569	− 122.0	LH0
	7	0.33	0.544	− 116.0	HH2	0.19	0.404	− 122.0	LH0
	Total	5.06	0.564			5.67	0.324		
77	0	2.28	0.569	− 7.22	HH0	2.39	0.144	5.58	HH0
	1	1.24	0.309	− 7.22	HH0	1.84	0.111	5.58	HH0
	2	0.61	0.887	− 19.7	LH0	0.47	0.267	− 13.3	HH1
	3	0.46	0.664	− 19.7	LH0	0.41	0.238	− 13.3	HH1
	4	0.25	0.399	− 20.4	HH1	0.02	0.557	− 38.9	HH2
	5	0.21	0.333	− 20.4	HH1	0.01	0.383	− 38.9	HH2
	6	0.12	0.495	− 26.5	HH2	0.00	0.715	− 53.7	LH0
	7	0.09	0.375	− 26.5	HH2	0.00	0.210	− 53.7	LH0
	Total	5.27	0.578			5.15	0.154		

at the top of the bands. For unstrained MODFET's where the top of the bands are very flat due to strong interactions between the light- and heavy-hole states, reduced temperatures do not mean lower effective masses. For strained MODFET's, the band tops are very light thus, lower temperature can mean significantly lower hole effective masses. We note that the low-temperature masses which we predict for the two HH0 states are close to the masses which Stormer *et al.* measured using cyclotron resonance techniques in the lattice-matched system.[9] Also, the extent of the decrease in the effective mass due to strain which we calculate is consistent with the experimental work by Jones *et al.*[10]

Our calculations clearly show that strained p-MODFET's should have much better performance than lattice-matched p-MODFET's. The p-MODFET problem is quite complicated, and there has been little experimental work to characterize these devices. The model described in this letter is quite powerful for modeling the strained p-channel MODFET, and can be used to study the effects of material parameters and device dimensions as well as gate voltage control over operation of the device. The model should prove quite useful in the design and optimization of these devices.

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